were to be extended from point to space groups, and the contracted groups have some common features with the 'P-symmetry groups' of Zamorzaev (1967). Let us also mention the classification work of Bohm & Dornberger-Schiff (1967) in which the augmented matrices represent either the contracted groups or ordinary subperiodic groups with respect to an origin which lies in the hyperplane they leave invariant [the matrices given in that work are not general enough to express subperiodic groups with respect to any chosen origin in $E(n)$].

The site-point groups of the Euclidean space may be also considered as the simplest kind of subperiodic group - groups with trivial translation subgroup. It is well known that space groups may be considered as extensions of translation subgroups by point groups (Ascher & Janner, 1965; 1968/69). Analogously, reducible space groups may be considered as extensions of their partial translation subgroups by the corresponding factor groups - the subperiodic groups. It is again an advantage to use the contracted subperiodic groups in such an approach. There are far-reaching analogies in the consideration of space groups as extensions by subperiodic groups with the ordinary consideration of these groups as extensions by point groups.

The first immediate consequence of the factorization theorem is, however, the fact that we can classify reducible space groups into subperiodic classes. This will be the subject of our subsequent paper.

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Subperiodic Classes of Reducible Space Groups

BY VOJTĚCH KOPSKÝ

Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, *POB* 24, 18040 *Praha* 8, *Czechoslovakia*

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Abstract

Classification of reducible space groups into pairs of complementary subperiodic classes with respect to various reductions is introduced and analysed. This classification is finer than the classification into geometric classes and it intersects with the classification into arithmetic classes. It is proved that an intersection theorem holds for those classes which correspond to Z decomposition of the translation subgroups of the reducible space groups and then symmorphic representatives of subperiodic classes of reducible space groups are introduced in analogy with the ordinary concept of symmorphic space groups. In particular, it is shown that the symmorphic space group is a symmorphic representative of subperiodic classes, defined by complementary symmorphic subperiodic groups. In cases of Z reductions it is shown that the pair of complementary subperiodic classes may define none, one or several space groups; if one such group belongs to these classes, then also a set of groups which differ by shifts in space does. These shifts are determined with translation normalizers. Further ramifications and possible use of the theory are discussed.

1. Introduction

As we have shown in a previous paper (Kopský, 1989), reducible space groups can be factorized by their partial translation subgroups and the resulting groups can be interpreted as subperiodic groups. *Vice*

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versa, we can accordingly assign reducible space groups to various subperiodic classes. The subperiodic groups which define these classes belong themselves to the same geometric classes as the reducible space groups. Each reducible space group can be assigned to at least one pair of subperiodic classes. This is exactly the case when the point group G admits just one, that is an orthogonal reduction class. Generally, the space group is assigned to various pairs of subperiodic classes, depending on the reduction with respect to which we perform the factorization. The number of such classifications is finite if the group G admits only orthogonal reducibility, infinite if it admits inclined reductions.

Different reducible space groups of the same type have technically different reductions and their subperiodic classes are accordingly defined by different contracted subperiodic groups. We show in the next section how to reduce the problem to representatives of space-group types through affine equivalence. In this connection we also discuss the relationship of enantiomorphism of reducible space groups with enantiomorphism of corresponding subperiodic groups.

Then we discuss the problem of determination of space groups which belong to various subperiodic classes. In particular, we study the relationship between pairs of complementary contracted subperiodic groups and space groups which belong to thus defined subperiodic classes. We prove an intersection theorem which says that reducible space groups, the translation subgroup of which is a direct sum of translation subgroups (Z decomposition) of two complementary subperiodic groups, lie on the intersections of these classes. In this connection we also define the symmorphic representatives of subperiodic classes and discuss their geometrical meaning.

Further, we investigate the case when translation subgroups of subperiodic groups which define subperiodic classes couple into a subdirect sum (Z reduction) which determines the translation subgroup of a space group. We show that in such a case one space group, which belongs to the two subperiodic classes, generally defines a set of space groups which belong to the same pair of classes and which differ only by a shift in space. It is shown how to determine these shifts with translation normalizers.

The paper closes with a discussion of the relationship of the factorization procedure and of subperiodic classes to other problems of space-group theory, especially in the theory of lattices of normal subgroups of space groups and in the so-called scanning of subperiodic groups.

Since the present paper is a natural continuation of the previous one (Kopský, 1989), we use the terminology and concepts used there without referring to it; when we use formulae, definitions or theorems of that paper, we refer to them with roman number I.

2. Subperiodic classes of reducible space groups

In view of theorem I.2, we can classify reducible space groups into classes of subperiodic groups. If the point group G admits only one reduction of the space $V(T_G, Q)$, then the classification is unique; the space group belongs to two complementary subperiodic classes. If there are several or infinitely many reductions, then we must relate the classifications to individual reductions.

Definition 1: Let $\mathscr{G}$ be a reducible space group, $V(T_G, Q) = V_1(k, Q) \oplus V_2(h, Q)$ a certain Q reduction and $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$ the homomorphisms, defined by relations (I.10) or (I.10b). Then we say that the group $\mathscr{G}$ belongs to subperiodic classes $\mathscr{L} = \boldsymbol{\sigma}_1(\mathscr{G})$, $\mathscr{R} = \boldsymbol{\sigma}_2(\mathscr{G})$ with respect to this reduction.

This definition concerns a certain space group $\mathscr{G}$ and the resulting classes are given by certain subperiodic groups or contracted subperiodic groups. We would, of course, prefer to have a classification for all space-group types. It is intuitively clear that, for two reducible space groups of the same type, there exist equivalent reductions, with respect to which the space groups are classified into subperiodic classes of the same type of subperiodic groups. It is therefore sufficient, for the purposes of tabular record, to find the reductions and classifications for one reference group of each space-group type and to show how to transform this information to other space groups of this type.

To find the relationships between the classification of various space groups of the same type with respect to equivalent reductions, it is suitable to consider affine conjugation as the operation of the affine group Af(n) on the reference group $\mathscr{G}$ of the space-group type. We denote by

$$\mathscr{G}_\alpha(\boldsymbol{\tau}) = \alpha_P(\boldsymbol{\tau}) \,.\, \mathscr{G} = \{\alpha\,|\,\boldsymbol{\tau}\}_P \mathscr{G} \{\alpha^{-1}\,|-\alpha^{-1}\boldsymbol{\tau}\}_P$$

the group which will be obtained from $\mathscr{G}$ by affine conjugation. The affine operation used in the conjugation consists of an operation which leaves invariant the point P chosen for the origin (deformation plus rotation), followed by translation $\boldsymbol{\tau}$ and it acts on the Euclidean space. Corresponding conjugation of the group $\mathscr{G}$ is written as an action of element of Af(n), considered as an inner automorphism of Af(n) [the affine group Af(n) has a trivial centre], on its subgroups. This provides a suitable formalism in which operators of pure translations may be denoted by $\varepsilon(\boldsymbol{\tau})$, multiplication of subsequently used automorphisms gives $\alpha_P(\boldsymbol{\tau})\beta_P(\boldsymbol{\mu}) = (\alpha\beta)_P(\boldsymbol{\tau} + \alpha\boldsymbol{\mu})$ and reciprocal to a given automorphism is $(\alpha_P(\boldsymbol{\tau}))^{-1} = (\alpha^{-1})_P(-\alpha^{-1}\boldsymbol{\tau})$. Let us now consider groups

$$\mathscr{G} = \{G, T_G, P, \mathbf{u}_G(g)\}, \qquad (1a)$$

$$\varepsilon(\boldsymbol{\tau})\mathscr{G}=\mathscr{G}(\boldsymbol{\tau})$$
$$=\{G, T_G, P, \mathbf{u}_G(g)+\boldsymbol{\varphi}(g,\boldsymbol{\tau})\}$$
$$=\{G, T_G, P+\boldsymbol{\tau}, \mathbf{u}_G(g)\}, \qquad (1b)$$
$$\alpha_P(\mathbf{0})\mathscr{G}=\mathscr{G}_\alpha=\{\alpha G\alpha^{-1}, \alpha T_G, P, \alpha\mathbf{u}_G(g)\}, \qquad (1c)$$
$$\alpha_P(\boldsymbol{\tau})\mathscr{G}=\mathscr{G}_\alpha(\boldsymbol{\tau})$$
$$=\{\alpha G\alpha^{-1}, \alpha T_G, P, \alpha\mathbf{u}_G(g)+\boldsymbol{\varphi}(\alpha g\alpha^{-1},\boldsymbol{\tau})\}$$
$$=\{\alpha G\alpha^{-1}, \alpha T_G, P+\boldsymbol{\tau}, \alpha\mathbf{u}_G(g)\} \qquad (1d)$$

and the group

$$\mathscr{G}_\alpha(\alpha\boldsymbol{\tau})=\{\alpha G\alpha^{-1}, \alpha T_G, P, \alpha\mathbf{u}_G(g)+\alpha\boldsymbol{\varphi}(g,\boldsymbol{\tau})\}$$
$$=\{\alpha G\alpha^{-1}, \alpha T_G, P+\alpha\boldsymbol{\tau}, \alpha\mathbf{u}_G(g)\}. \qquad (1e)$$

The first two groups differ only by a shift $\boldsymbol{\tau}$ and we can apply the same homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$ to them. We already know the result. It is $\boldsymbol{\sigma}_1(\mathscr{G}(\boldsymbol{\tau}))=\mathscr{L}(\boldsymbol{\tau}_1)$, $\boldsymbol{\sigma}_2(\mathscr{G}(\boldsymbol{\tau}))=\mathscr{R}(\boldsymbol{\tau}_2)$, so that the shift of the original group by $\boldsymbol{\tau}$ leads to the shift of its projections by projections of the shift $\boldsymbol{\tau}$ onto corresponding subspaces.

If the group G leaves invariant subspaces $V_1(k,R)$, $V_2(h,R)$, then the group $\alpha G\alpha^{-1}$ leaves invariant subspaces $\alpha V_1(k,R)$, $\alpha V_2(h,R)$. Also, if $V(T_G,Q)=V_1(k,Q)\oplus V_2(h,Q)$ is a Q reduction which implies Z reduction or Z decomposition, (I.3a) with (I.3b) or (I.3c), then $\alpha V(T_G,Q)=V(\alpha T_G,Q)=\alpha V_1(k,Q)\oplus\alpha V_2(h,Q)$ is a Q reduction, which implies Z reduction or Z decomposition of the group $\alpha(T_G)$ into either subdirect or direct sum of groups $\alpha(T^0_{G1})$, $\alpha(T^0_{G2})$ and the projections σ_1, σ_2 in (I.3b) have to be replaced by $\sigma_{\alpha1}=\alpha\sigma_1\alpha^{-1}$, $\sigma_{\alpha2}=\alpha\sigma_2\alpha^{-1}$. If α is just an isotropic deformation of the subspaces $V_1(k,R)$, $V_2(h,R)$, in which all vectors of $V_1(k,R)$ are multiplied by a common factor, all vectors of $V_2(h,R)$ by another common factor, then the R reduction will not change and the transformed groups $\mathscr{G}_\alpha(\boldsymbol{\tau})$ can be mapped into the same general contracted subperiodic groups as the group $\mathscr{G}$.

Definition 2: The reduction $V(n,R)=V_1(k,R)\oplus V_2(h,R)$, associated with the group $\mathscr{G}$, and the reduction $V(n,R)=\alpha V_1(k,R)\oplus\alpha V_2(h,R)$, associated with the group $\mathscr{G}_\alpha$, are said to be equivalent.

It is easy to show that, if T_{G1}, T_{G2} are partial translation subgroups of groups $\mathscr{G}(\boldsymbol{\tau})$, then $\alpha(T_{G1})$, $\alpha(T_{G2})$ are partial translation subgroups of groups $\mathscr{G}_\alpha(\boldsymbol{\tau})$ and that the factor groups $\mathscr{G}_\alpha(\boldsymbol{\tau})/\alpha(T_{G1})$, $\mathscr{G}_\alpha(\boldsymbol{\tau})/\alpha(T_{G2})$ are isomorphic with $\mathscr{G}(\boldsymbol{\tau})/T_{G1}$, $\mathscr{G}(\boldsymbol{\tau})/T_{G2}$, respectively. We want, however, to find also the homomorphisms $\boldsymbol{\sigma}_{\alpha1}, \boldsymbol{\sigma}_{\alpha2}$ which map the space groups $\mathscr{G}_\alpha(\boldsymbol{\tau})$ onto contracted subperiodic groups of appropriate geometrical meaning, which can be interpreted as projections of space groups.

It is only a problem of a small calculation to do that if we work with mapping on subperiodic groups of the Euclidean space, which leave invariant hyperplanes $(P, \alpha V_1(k,R))$, $(P, \alpha V_2(h,R))$, because these are also subgroups of the affine group and operators $\alpha_P(\boldsymbol{\tau})$ can be applied to them. We define again the homomorphisms by $\boldsymbol{\sigma}_{\alpha i}\{\alpha g\alpha^{-1}|\mathbf{t}\}_P=\{\alpha g\alpha^{-1}|\sigma_{\alpha i}(\mathbf{t})\}_P=\{\alpha g\alpha^{-1}|\mathbf{t}_i\}_P$. From relations

$$\boldsymbol{\sigma}_{\alpha i}\alpha_P(\boldsymbol{\tau})\{g|\mathbf{t}\}_P$$
$$=\boldsymbol{\sigma}_{\alpha i}\{\alpha g\alpha^{-1}|\alpha\mathbf{t}+\boldsymbol{\varphi}(\alpha g\alpha^{-1},\boldsymbol{\tau})\}_P$$
$$=\{\alpha g\alpha^{-1}|\sigma_{\alpha i}\alpha\mathbf{t}+\sigma_{\alpha i}(\boldsymbol{\tau}-\alpha g\alpha^{-1}\,.\,\boldsymbol{\tau})\}_P$$
$$=\{\alpha g\alpha^{-1}|\alpha\sigma_i(\mathbf{t})+\boldsymbol{\varphi}(\alpha g\alpha^{-1},\boldsymbol{\tau}_{\alpha i})\}_P$$
$$=\alpha_P(\boldsymbol{\tau}_{\alpha i})\{g|\sigma_i(\mathbf{t})\}_P$$
$$=\alpha_P(\boldsymbol{\tau}_{\alpha i})\boldsymbol{\sigma}_i\{g|\mathbf{t}\}_P,$$

which can be applied to any element of $\mathscr{E}_1(k)\times\mathscr{E}_2(h)$, we get a very useful relation between homomorphisms and automorphisms:

$$\boldsymbol{\sigma}_{\alpha i}\alpha_P(\boldsymbol{\tau})=\alpha_P(\boldsymbol{\tau}_{\alpha i})\boldsymbol{\sigma}_i, \qquad i=1,2. \qquad (2)$$

Applying both sides of this relation to a group $\mathscr{G}$, we get

$$\boldsymbol{\sigma}_{\alpha i}\alpha_P(\boldsymbol{\tau})\mathscr{G}=\boldsymbol{\sigma}_{\alpha i}(\mathscr{G}_\alpha(\boldsymbol{\tau}))$$
$$=\alpha_P(\boldsymbol{\tau}_{\alpha i})\boldsymbol{\sigma}_i(\mathscr{G})$$
$$=\begin{cases}\alpha_P(\boldsymbol{\tau}_{\alpha1})\mathscr{L}=\mathscr{L}_\alpha(\boldsymbol{\tau}_{\alpha1})\\ \alpha_P(\boldsymbol{\tau}_{\alpha2})\mathscr{R}=\mathscr{R}_\alpha(\boldsymbol{\tau}_{\alpha2}),\end{cases}$$

where $\boldsymbol{\tau}_{\alpha1}, \boldsymbol{\tau}_{\alpha2}$ are projections of $\boldsymbol{\tau}$ to $\alpha V_1(k,R)$, $\alpha V_2(h,R)$. Notice that application of homomorphisms $\boldsymbol{\sigma}_{\alpha1}, \boldsymbol{\sigma}_{\alpha2}$ to the group (1e), which differs from (1d) in the order in which $\alpha_P(\mathbf{0})$ and $\varepsilon(\boldsymbol{\tau})$ are applied, gives

$$\boldsymbol{\sigma}_{\alpha1}(\mathscr{G}_\alpha(\alpha\boldsymbol{\tau}))=\mathscr{L}_\alpha(\alpha\boldsymbol{\tau}_1),$$
$$\boldsymbol{\sigma}_{\alpha2}(\mathscr{G}_\alpha(\alpha\boldsymbol{\tau}))=\mathscr{R}_\alpha(\alpha\boldsymbol{\tau}_2),$$

where $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2$ are projections of $\boldsymbol{\tau}$ to $V_1(k,R)$, $V_2(h,R)$.

These results are again tied up with the choice of the point P, which can be added as an index to homomorphisms $\boldsymbol{\sigma}_{\alpha i}$. This consideration shows, however, how to choose the general contracted subperiodic groups and the homomorphisms into these groups. We have to introduce again Cartesian products $E_{\alpha1}(k)\times\alpha V_2(h,R)$, $\alpha V_1(k,R)\times E_{\alpha2}(h)$, where $\alpha V_1(k,R)$, $\alpha V_2(h,R)$ are difference spaces of $E_{\alpha1}(k)$, $E_{\alpha2}(h)$, respectively and $\mathscr{E}_{\alpha1}(k)\times\mathscr{O}_{\alpha2}(h)$, $\mathscr{O}_{\alpha1}(k)\times\mathscr{E}_{\alpha2}(h)$ are the general contracted subperiodic groups acting on these spaces. The groups $\mathscr{O}_{\alpha1}(k)=\alpha\mathscr{O}_1(k)\alpha^{-1}$, $\mathscr{O}_{\alpha2}(h)=\alpha\mathscr{O}_2(h)\alpha^{-1}$ are here the orthogonal groups on $\alpha V_1(k,R)$, $\alpha V_2(h,R)$ and the elements of contracted groups are $[\alpha g\alpha^{-1}|\alpha\mathbf{t}_1]_P$, $\langle\alpha g\alpha^{-1}|\alpha\mathbf{t}_2\rangle_P$. If we now define homomorphisms $\boldsymbol{\sigma}_{\alpha1}$, $\boldsymbol{\sigma}_{\alpha2}$ by

$$\boldsymbol{\sigma}_{\alpha1}\{\alpha g\alpha^{-1}|\mathbf{t}\}_P=[\alpha g\alpha^{-1}|\sigma_{\alpha1}(\mathbf{t})]_P=[\alpha g\alpha^{-1}|\alpha\mathbf{t}_1]_P;$$
$$\boldsymbol{\sigma}_{\alpha2}\{\alpha g\alpha^{-1}|\mathbf{t}\}_P=\langle\alpha g\alpha^{-1}|\sigma_{\alpha2}(\mathbf{t})\rangle_P=\langle\alpha g\alpha^{-1}|\alpha\mathbf{t}_2\rangle_P,$$

we can prove relations (2) in exactly the same way as we did for homomorphisms onto ordinary subperiodic groups. We then get, in the notation for contracted subperiodic groups,

$$\begin{aligned}\boldsymbol{\sigma}_{\alpha 1}(\mathscr{G}_\alpha(\boldsymbol{\tau})) &= \mathscr{L}_\alpha(\boldsymbol{\tau}_{\alpha 1})\\ &= [\alpha G\alpha^{-1}, \alpha T^0_{G1}, P_1+\boldsymbol{\tau}_{\alpha 1}, \alpha \mathbf{u}_{G1}(g)],\\ \boldsymbol{\sigma}_{\alpha 2}(\mathscr{G}_\alpha(\boldsymbol{\tau})) &= \mathscr{R}_\alpha(\boldsymbol{\tau}_{\alpha 2})\\ &= \langle \alpha G\alpha^{-1}, \alpha T^0_{G2}, P_2+\boldsymbol{\tau}_{\alpha 2}, \alpha \mathbf{u}_{G2}(g)\rangle.\end{aligned} \tag{3}$$

We can formulate these results as:

Theorem 1 (*Equivalence of classifications*): If a reducible space group $\mathscr{G}$ belongs to complementary subperiodic classes $\mathscr{L}$ and $\mathscr{R}$ with respect to a reduction $V(n, R) = V_1(k, R) \oplus V_2(h, R)$, then the group $\mathscr{G}_\alpha(\boldsymbol{\tau})$ is also reducible and belongs to complementary subperiodic classes $\mathscr{L}_\alpha(\boldsymbol{\tau}_{\alpha 1})$ and $\mathscr{R}_\alpha(\boldsymbol{\tau}_{\alpha 2})$ with respect to reduction $V(n, R) = \alpha V_1(k, R) \oplus \alpha V_2(h, R)$.

We have performed all these considerations within the realm of affine groups, so that groups $\mathscr{G}_\alpha(\boldsymbol{\tau})$ are not necessarily Euclidean space groups. Actually, the whole reducibility theory can be developed from the beginning for affine space groups under which we understand any affine conjugates of Euclidean space groups. If we want to remain within the Euclidean space groups, it is sufficient to assume that $\mathscr{G}$ is Euclidean and $\alpha_P(\boldsymbol{\tau})$ such that the group $\alpha G\alpha^{-1}$ is orthogonal (assuming G itself is orthogonal).

Enantiomorphism

The affine group Af(n) has a halving subgroup Af$^+(n)$, consisting of those affine operations of which the linear constituents belong to the group $G^+V(n)$, the halving subgroup of the general linear group $GV(n)$ of operators on $V(n)$, which consists only of linear operators with positive determinant. We shall use the symbol α for the elements of these groups now, reserving m and $m\alpha$ or αm for elements of cosets, for which the determinants are negative. The translational parts can be disregarded in consideration of enantiomorphism, so that we can neglect the difference between affine operations and corresponding linear operators.

Now, an affine class defined by a group $\mathscr{G}$ either splits or does not split into a pair of proper affine classes, called enantiomorphic pair. If for an arbitrarily chosen m there exists α such that $\mathscr{G}_m = \mathscr{G}_\alpha$, then for each m there exists some α such that the groups coincide and enantiomorphism does not occur. If for some m there does not exist any such α, then such an α exists for none of the m and enantiomorphism occurs – elements of Af$^+(n)$ send the group to one of the proper classes, the elements of the coset to the other. There are simple criteria: (i) enantiomorphism occurs when the affine normalizer of $\mathscr{G}$ lies completely in Af$^+(n)$, (ii) there is no enantiomorphism if the affine normalizer of $\mathscr{G}$ contains at least one element of $m\,.\,$Af$^+(n)$. Despite the simplicity of these criteria, the occurrence of enantiomorphism in arbitrary dimensions has not been completely analysed. According to those criteria, we have to look up whether there exists an m such that the group $\mathscr{G}_m = \{mGm^{-1}, mT_G, P, m\mathbf{u}_G(g)\}$ coincides with the group $\mathscr{G} = \{G, T_G, P, \mathbf{u}_G(g)\}$. Then we have three possible kinds of enantiomorphism:

(i) *geometric enantiomorphism*: if the linear normalizer of G lies completely in $G^+V(n)$, then mGm^{-1} does not coincide with G for any m;

(ii) *arithmetic enantiomorphism*: if $mGm^{-1} = G$ for some m, but for none of them $mT_G = T_G$;

(iii) *screw enantiomorphism*: there exists m for which $mGm^{-1} = G$ and $mT_G = T_G$ but for some $\mathbf{u}_G(g)$ the systems of nonprimitive translations $\mathbf{u}_G(g)$ and $m\mathbf{u}_G(g)$ are not equivalent.

It would be interesting to find out how enantiomorphism of reducible space groups depends on the enantiomorphisms of its subperiodic classes. Geometric enantiomorphism may occur only in spaces of even dimensions because the complete inversion always has the property $iGi^{-1} = G$ and in spaces of odd dimensions it belongs to the coset $mG^+V(n)$. This enantiomorphism is then common for all groups of a geometric class, including the subperiodic ones. We do not know any examples of arithmetic enantiomorphism. Geometric enantiomorphism has been found for the four-dimensional cases in the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978); it leads to enantiomorphism of arithmetic classes but there is no case where arithmetic enantiomorphism occurs. Screw enantiomorphism occurs in three dimensions, where 10 of the 11 pairs are reducible. Enantiomorphism of space groups is, in these cases, connected with enantiomorphism of their rod classes. It seems that, in general, screw enantiomorphism of space groups implies screw enantiomorphism in at least one of the subperiodic classes with respect to any possible reduction but we have not proved this so far.

3. Inverse problems in the factorization process and refinement of space-group classification

Up to now we have considered situations when a reducible space group is known or given and we are looking for subperiodic classes to which it belongs with respect to various possible reductions. This is one side of the relationship between reducible space groups and contracted subperiodic groups. Inverse problems may be described as those in which we are concerned with the extent to which the space groups are determined on the grounds of various items of information on their subperiodic classes.

Classification of reducible space groups into subperiodic classes refines the accepted classification scheme into geometric and arithmetic classes with which we are familiar. Actually, a finer classification is desirable even within the geometric class. We shall first see how to refine the classification of space and subperiodic groups of a given geometric class.

3.1. *Space groups with the same point group*

The point group G defines a geometric class. This, however, includes all space groups which have, as their point group, any of the conjugates of G in $\mathcal{O}(n)$. Since fixing of G means geometrically fixing the 'orientation of the group', we shall say that the set of all space groups with a given G forms an 'oriented geometric class'.

As a next step we have to look for all possible G-invariant translation subgroups T_G (we assume that G is crystallographic and hence we look only for discrete groups T_G). Any pair (G, T_G) then defines an arithmetic class; since we consider only a fixed group G, we shall use the term 'oriented arithmetic class' for space groups of the same arithmetic class with fixed group G. Again there is freedom in the choice of translation subgroups T_G within the oriented arithmetic class. This is the freedom in the choice of lattice parameters. The set of space groups with the same pair (G, T_G) in which not only G but also T_G is fixed may then be called an oriented 'arithmetic class with fixed parameters'. We shall use the symbol $\{G, T_G\}$ for this set of groups and reserve the symbol (G, T_G) for the whole arithmetic class.

The groups within the same class $\{G, T_G\}$ then differ by systems of nonprimitive translations with respect to a given origin P. A certain space group $\mathcal{G}=\{G, T_G, P, \mathbf{u}_G(g)\}$ of the class $\{G, T_G\}$ generates a set of groups

$$\mathcal{G}(\boldsymbol{\tau})=\{G, T_G, P, \mathbf{u}_G(g)+\boldsymbol{\varphi}(g, \boldsymbol{\tau})\}, \qquad (4a)$$

which differ only by a shift $\boldsymbol{\tau}$ from $\mathcal{G}$. Further, $\mathcal{G}(\boldsymbol{\tau})=\mathcal{G}$ if and only if $\boldsymbol{\varphi}(g, \boldsymbol{\tau})=\mathbf{0}$ (mod T_G) for all $g\in G$. Solutions of the last congruences form a translation group, which is common for all groups of a given arithmetic class $\{G, T_G\}$. This group, denoted by $T_N\{G, T_G\}$, is the translation subgroup of both affine and Euclidean normalizers of groups of the arithmetic class $\{G, T_G\}$. We call it the *translation normalizer* of the group $\mathcal{G}$ (Kopský, 1990). Let us remark that the significance of translation normalizers escaped the attention of crystallographers as previously did the importance of normalizers at all, though they have been more or less explicitly used [Boyle & Lawrenson (1973); Giacovazzo (1974); translation subgroups of Cheshire groups by Hirshfeld (1968)]. They are mentioned in the last edition of *International Tables for Crystallography* (Hahn, 1987) as translation subgroups of Euclidean and affine normalizers and since the latter are known and tabulated in this edition, there seems to be no necessity to be concerned with the translation normalizers. This is, however, only an impression which occurs partly because both Euclidean and affine normalizers of groups up to three dimensions can be easily guessed from their diagrams. The translation normalizers are an important theoretical tool themselves (we shall see one example of their application below) and their calculation would be the first natural and unavoidable step in the calculation of Euclidean or affine normalizers in general dimensions. They are also known under the name of weight groups (Schwarzenberger, 1980; Maxwell, 1975).

Thus, it is $\mathcal{G}(\boldsymbol{\tau})=\mathcal{G}$ as long as $\boldsymbol{\tau}\in T_N\{G, T_G\}$. It is therefore meaningful to distinguish only the groups $\mathcal{G}(\boldsymbol{\tau})$ for which $\boldsymbol{\tau}$ are representatives in coset resolution of $V(n, R)$ with respect to $T_N\{G, T_G\}$.

Further, we choose a certain system of nonprimitive translations $\mathbf{u}_G^{(\alpha)}(g)$ and accordingly a certain space group $\mathcal{G}^{(\alpha)}=\{G, T_G, P, \mathbf{u}_G^{(\alpha)}(g)\}$ as a representative in each set of translationally conjugate space groups. Then every space group of the arithmetic class $\{G, T_G\}$ with fixed orientation of G and lattice parameters of T_G is one of the groups $\mathcal{G}^{(\alpha)}(\boldsymbol{\tau})$. It is possible to choose the systems of nonprimitive translations in such a way that they will themselves form a group under addition modulo T_G (we ask the reader to believe this statement without proof) and then we can introduce formal multiplication of space groups in the class $\{G, T_G\}$:

$$\mathcal{G}^{(\alpha)}(\boldsymbol{\tau})\,.\,\mathcal{G}^{(\beta)}(\boldsymbol{\mu})=\mathcal{G}^{(\gamma)}(\boldsymbol{\nu}) \qquad (5a)$$

if

$$\mathbf{u}_G^{(\alpha)}(g)+\mathbf{u}_G^{(\beta)}(g)=\mathbf{u}_G^{(\gamma)}(g) \ (\mathrm{mod}\ T_G)$$

and

$$\boldsymbol{\tau}+\boldsymbol{\mu}=\boldsymbol{\nu} \ (\mathrm{mod}\ T_N\{G, T_G\}).$$

We call this law the *Baer multiplication* of space groups.

Actually, the sets $\mathcal{G}^{(\alpha)}(\boldsymbol{\tau})$ with the labels (α) define so-called extension classes which correspond to the elements of the second cohomology group $H^2\{G, T_G\}$ (Ascher & Janner, 1965, 1968/69).

Let us finally recall that the space groups with a trivial (either vanishing or equal to shift function) system of nonprimitive translations are the so-called symmorphic groups of the arithmetic class $\{G, T_G\}$. These groups correspond to the unit element of the group $H^2(G, T_G)$.

3.2. *Contracted (and ordinary) subperiodic groups with a given point group*

It is intuitively clear (and we shall prove it soon) that every contracted subperiodic group of a given geometric class G appears as a factor group to some space groups of the same geometric class. Subperiodic groups also form geometric and oriented geometric, arithmetic and oriented arithmetic classes as well as oriented arithmetic classes with fixed parameters. Within a given oriented geometric class, the subperiodic groups differ by the G-invariant subspaces $V_1(k, R)$ spanned by their translation subgroups T_{G1}. If the group G admits only orthogonal reductions, there is a finite number of possible G-invariant subspaces, otherwise there are infinitely many. The dimension k of $V_1(k, R)$ together with the total dimension n determines the kind of subperiodic group (frieze, layer, rod or magnetic groups to name those which are already in use). The action of G on T_{G1} determines an arithmetic class; if orientation of G and parameters of T_{G1} are fixed, we again say that the groups with the same G, T_{G1} form an oriented arithmetic class $[G, T_{G1}]$ with fixed parameters. We shall distinguish arithmetic classes of contracted subperiodic groups by the same kinds of brackets we use for their Seitz symbols. Thus $\{G, T_G\}$ will mean an oriented arithmetic class with fixed parameters for the ordinary subperiodic groups which belong to the contracted class $[G, T_{G1}]$. Again we may reserve the symbol (G, T_{G1}) for the whole arithmetic class.

Within the arithmetic class $[G, T_{G1}]$ we can use the same scheme as in the arithmetic class $\{G, T_G\}$ of space groups. Hence each group $\mathscr{L} = [G, T_{G1}, P_1, \mathbf{u}_{G1}(g)]$ generates a set of translationally conjugate groups

$$\mathscr{L}(\boldsymbol{\tau}_1) = [G, T_{G1}, P_1, \mathbf{u}_{G1}(g) + \boldsymbol{\varphi}(g, \boldsymbol{\tau}_1)] \qquad (4b)$$

and the translation normalizer $T_N[G, T_{G1}]$ determines all vectors of $V_1(k, R)$ for which $\mathscr{L}(\boldsymbol{\tau}_1) = \mathscr{L}$. We use the same kind of brackets in the symbol of a normalizer as in the symbols for groups and arithmetic classes; here the square brackets indicate that we consider only shifts in $V_1(k, R)$ as it is natural for contracted subperiodic groups. This should be distinguished from the translation normalizer $T_N\{G, T_{G1}\}$ which will be the normalizer of ordinary subperiodic groups of the arithmetic class $\{G, T_{G1}\}$ in $E(n)$ and where, accordingly, all vectors of $V(n, R)$ will be considered.

Again we can choose a representative system of nonprimitive translations $\mathbf{u}_{G1}^{(\alpha_1)}(g)$ and the respective group $\mathscr{L}^{(\alpha_1)}$ in each set of translationally conjugate groups of the class $[G, T_{G1}]$, again we can choose the representatives in such a way that they themselves form a group under addition mod T_{G1} and again we can introduce Baer multiplication:

$$\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1) \,.\, \mathscr{L}^{(\beta_1)}(\boldsymbol{\mu}_1) = \mathscr{L}^{(\gamma_1)}(\boldsymbol{\nu}_1) \qquad (5b)$$

for

$$\mathbf{u}_{G1}^{(\alpha_1)}(g) + \mathbf{u}_{G1}^{(\beta_1)}(g) = \mathbf{u}_{G1}^{(\gamma_1)}(g) \ (\text{mod } T_{G1})$$

and

$$\boldsymbol{\tau}_1 + \boldsymbol{\mu}_1 = \boldsymbol{\nu}_1 \ (\text{mod } T_N[G, T_{G1}]).$$

The groups for which the system of nonprimitive translations is trivial, *i.e.* either vanishing or equal to the shift function, are again the symmorphic groups of the arithmetic class $[G, T_{G1}]$. The same scheme naturally holds also for the complementary contracted subperiodic groups, for which we introduce oriented classes $\langle G, T_{G2}\rangle$ with fixed parameters.

3.3. *Inverse problems connected with subperiodic classes*

Now we shall see to what extent various information on subperiodic classes determines a space group. There are two main situations:

1. We assume that a certain admissible reduction $V(n, R) = V_1(k, R) \oplus V_2(h, R)$ is given. The basic problem is then: Given two subperiodic groups $\mathscr{L}$ and $\mathscr{R}$ with translation subgroups in $V_1(k, R)$, $V_2(h, R)$, respectively, what space groups belong to their subperiodic classes with respect to this reduction? We can extend the problem and include certain suitable sets of subperiodic groups instead of one pair (for example all the arithmetic classes).

2. We assume that only one of the G-invariant subspaces is specified, say the $V_1(k, R)$, and the basic problem is then the determination of space groups which belong to a certain subperiodic class, defined by the contracted group, the translation subgroup of which lies in $V_1(k, R)$. Again we can extend the problem to consider space groups corresponding to a wider set of subperiodic groups (here we have also the arithmetic class in mind).

There are the following differences in the two problems: In the first one both homomorphisms σ_1 and σ_2 are specified from the beginning. In the second there are two possibilities: The subspace $V_1(k, R)$ defines uniquely the G-invariant complement $V_2(h, R)$ and hence both homomorphisms σ_1, σ_2 only if the resulting reduction is of orthogonal class. But the space $V_1(k, R)$ itself already determines whether the reduction class is orthogonal or inclined. If it is orthogonal, then the complement and hence also the homomorphisms are already defined by $V_1(k, R)$. In the case of inclined reductions there remains a certain freedom in the choice of the G-invariant complementary subspace and hence in the choice of homomorphisms σ_1, σ_2.

There is also a second difference in the two situations. In the first of them we assume also that both complementary subperiodic classes are specified. In the second we specify only one of the subperiodic classes. The choice of the complementary subspace in case of inclined reductions is a part of the specification of the complementary subperiodic group. In addition, we can further specify the arithmetic class of this group and finally the (lattice) parameters of this class.

4. Space groups on the intersection of subperiodic classes

For the sake of brevity, we shall now use the words geometric and arithmetic class in the meaning of oriented geometric and of oriented arithmetic class with fixed parameters. Both situations described in the preceding subsection then boil down to the following:

Given arithmetic classes $[G, T_{G1}]$ and $\langle G, T_{G2}\rangle$ of complementary contracted subperiodic groups; what space groups belong to corresponding subperiodic classes?

First of all, the arithmetic classes $[G, T_{G1}], \langle G, T_{G2}\rangle$ determine arithmetic classes $\{G, T_G\}$ of space groups which are candidates for consideration. The direct sum $T_G = T_{G1} \oplus T_{G2}$ is always G invariant if the components are, so that we have at once the arithmetic class $\{G, T_G\}$, which corresponds to the Z-decomposable case with respect to the reduction defined by spaces spanned by T_{G1}, T_{G2}. As we shall see, this case leads to a particularly simple and powerful result.

Further, there exist arithmetic classes $\{G, T_G\}$ with G-invariant translation groups T_G which are subdirect sums of groups T_{G1}, T_{G2}; these are now the groups we have usually supplied with superscripts 0. We do not know any general algorithm for the construction of such groups, especially in the case of inclined reduction. This belongs to one of the problems of integral (Z) representations which are, as far as we know, not yet completely solved. For up to four dimensions we know, however, all possible solutions. We shall restrict our consideration of these cases to a proof of one theorem which might be useful.

4.1. *Z-decomposable cases: intersection theorem and symmorphic representatives of subperiodic classes*

In the case when arithmetic class $\{G, T_G\}$ of reducible space groups is Z decomposable into arithmetic classes $[G, T_{G1}], \langle G, T_{G2}\rangle$, we have an elegant solution given by the following:

Theorem 2 (*Intersection theorem*): Let $[G, T_{G1}]$ and $\langle G, T_{G2}\rangle$ be arithmetic classes of contracted subperiodic groups and $\{G, T_G\}$ an arithmetic class of space groups, for which T_G is the direct sum of T_{G1}, T_{G2}. Then there is a one-to-one correspondence between space groups of the class $\{G, T_G\}$ and pairs of contracted subperiodic groups of arithmetic classes $[G, T_{G1}]$, $\langle G, T_{G2}\rangle$, given by $\mathscr{G} \leftrightarrow [\boldsymbol{\sigma}_1(\mathscr{G}), \boldsymbol{\sigma}_2(\mathscr{G})]$.

Proof: The groups T_{G1}, T_{G2} define the G-invariant subspaces and hence the homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$. These homomorphisms assign to each space group of the class $\{G, T_G\}$ exactly a unique pair of contracted groups of classes $[G, T_{G1}]$, $\langle G, T_{G2}\rangle$ by the factorization theorem. Let us now show that the opposite is also true. We shall use labels α_1, α_2 for sets of translationally conjugate groups $\mathscr{L}, \mathscr{R}$ respectively, indicating by labels $\alpha_1 = 1$ or $\alpha_2 = 1$ that either $\mathscr{L}$ or $\mathscr{R}$ is symmorphic.

If we now take a group $\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1)$ of the class $[G, T_{G1}]$, then its system of nonprimitive translations satisfies Frobenius congruences mod T_{G1}. But T_{G1} is a subgroup of T_G and hence the same system of nonprimitive translations satisfies also Frobenius congruences mod T_G. There exists therefore a space group of the class $\{G, T_G\}$ with the same system of nonprimitive translations as the group $\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1)$; we shall denote it by $\mathscr{G}^{(\alpha_1,1)}(\boldsymbol{\tau}_1)$. Analogously there exist space groups $\mathscr{G}^{(1,\alpha_2)}(\boldsymbol{\tau}_2)$ which correspond in the same way to groups $\mathscr{R}^{(\alpha_2)}(\boldsymbol{\tau}_2)$. Finally, to a pair of groups $(\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1); \mathscr{R}^{(\alpha_2)}(\boldsymbol{\tau}_2))$ we shall assign that space group $\mathscr{G}^{(\alpha_1,\alpha_2)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)$, the system of nonprimitive translations of which will be the sum of the systems of nonprimitive translations of the two subperiodic groups. Hence we get the correspondence

$$\mathscr{G}^{(\alpha_1,\alpha_2)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2) \leftrightarrow (\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1); \mathscr{R}^{(\alpha_2)}(\boldsymbol{\tau}_2)), \quad (6)$$

in which pairs of groups on the right-hand side are images of groups on the left-hand side by homomorphisms $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$.

The groups $\mathscr{G}^{(\alpha_1,1)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)$ belong to subperiodic classes $\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1)$ and $\mathscr{R}^{(1)}(\boldsymbol{\tau}_2)$, the latter of which is symmorphic. The groups $\mathscr{G}^{(1,\alpha_2)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)$ belong to subperiodic classes $\mathscr{L}^{(1)}(\boldsymbol{\tau}_1)$, $\mathscr{R}^{(\alpha_2)}(\boldsymbol{\tau}_2)$, the first of which is symmorphic.

Definition 3: The groups $\mathscr{G}^{(\alpha_1,1)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)$ will be called the *symmorphic groups of subperiodic class* $\mathscr{L}^{(\alpha_1)}(\boldsymbol{\tau}_1)$, the groups $\mathscr{G}^{(1,\alpha_2)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)$ will be called the *symmorphic groups of subperiodic class* $\mathscr{R}^{(\alpha_2)}(\boldsymbol{\tau}_2)$. It is, perhaps, also suitable to use the wording *partially symmorphic* groups.

This terminology is justified by the fact that partially symmorphic groups have analogous properties to the usual symmorphic groups. There are three equivalent characteristics of ordinary symmorphic groups: (1) Their systems of nonprimitive translations either vanish or are equal to the shift function with vector in $V(n, R)$. (2) There is a point in space (Wyckoff position) or rather a set of such points which exhibit the complete point symmetry of the space group. (3) The space group is a semidirect product (or split extension) of translation group and (by) the point group.

Analogously, the (partially) symmorphic space group of a certain subperiodic class has the following properties: (1) Its partial system of nonprimitive translations in complementary space either vanishes or equals the shift function. (2) There is a hyperplane (sets of hyperplanes) with directions generated by the translation subgroup of the subperiodic class which exhibits the full subperiodic symmetry with respect to the space group; such hyperplanes can also be distributed into Wyckoff sets. (3) The space group is a semidirect product (split extension) of partial translation subgroup in complementary space and (by) the subperiodic group.

Groups we have denoted by $\mathcal{G}^{(1,1)}(\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)$ are symmorphic groups of symmorphic subperiodic classes. We identify them easily as the symmorphic groups of the arithmetic class $\{G, T_G\}$.

The intersection theorem explains the algebraic origin of a fact long known to crystallographers (Cochran, 1952). It has been observed in connection with consideration of layer groups that to each layer group there corresponds a certain space group which has an identical diagram. This is now clearly seen in new editions of *International Tables for Crystallography* Vol. A (Hahn, 1987), where all settings of orthorhombic and monoclinic groups are presented. These space groups are just the symmorphic representatives of layer classes of reducible space groups. Analogously, we can find space groups which are representatives of rod classes.

4.2. *Z-reducible indecomposable cases*

The space groups defined by the intersection theorem do not generally exhaust all space groups which belong to subperiodic classes defined by groups of arithmetic classes $[G, T^0_{G1}]$, $\langle G, T^0_{G2}\rangle$. These pairs of arithmetic classes couple into arithmetic classes $\{G, T_G\}$ in which the group T_G is a subdirect sum of T^0_{G1} and T^0_{G2}. A dimension-independent analysis of these cases is still not quite satisfactory and it seems that it would be better to approach these cases in the language of group extensions. Two subperiodic groups $\mathcal{L}^{(\alpha_1)}$, $\mathcal{R}^{(\alpha_2)}$ do not necessarily define some space group of the Z-reducible arithmetic class $\{G, T_G\}$ if the latter is not decomposable into arithmetic classes $[G, T^0_{G1}]$, $\langle G, T^0_{G2}\rangle$. There may be, in general, no group on the intersection of such classes, one or several such groups, which may belong to the same or to different space-group types. A more detailed analysis is desirable, but we present one theorem which may be of interest.

Theorem 3: Let $\mathcal{G}$ be a space group of an arithmetic class $\{G, T_G\}$, in which the group T_G is Z reducible (not decomposable) into the subdirect sum of translation groups T^0_{G1}, T^0_{G2} of subperiodic arithmetic classes $[G, T^0_{G1}]$, $\langle G, T^0_{G2}\rangle$ and let this group belong to subperiodic classes $\mathcal{L}^{(\alpha_1)}$, $\mathcal{R}^{(\alpha_2)}$. Then all space groups $\mathcal{G}(\boldsymbol{\mu}_i)$, where $\boldsymbol{\mu}_i$ runs over the representatives in coset resolution of the direct sum of translation normalizers $T_N[G, T^0_{G1}]\oplus T_N\langle G, T^0_{G2}\rangle$ with respect to the translation normalizer $T_N\{G, T_G\}$, are distinct and belong to the same subperiodic classes.

Proof: It is a direct consequence of the factorization theorem that from $\mathcal{L}^{(\alpha_1)}=\boldsymbol{\sigma}_1(\mathcal{G}^{(\alpha)})$, $\mathcal{R}^{(\alpha_2)}=\boldsymbol{\sigma}_2(\mathcal{G}^{(\alpha)})$ follows $\boldsymbol{\sigma}_1(\mathcal{G}^{(\alpha)}(\boldsymbol{\tau}))=\mathcal{L}^{(\alpha_1)}(\boldsymbol{\tau}_1)$, $\boldsymbol{\sigma}_2(\mathcal{G}^{(\alpha)}(\boldsymbol{\tau}))=\mathcal{R}^{(\alpha_2)}(\boldsymbol{\tau}_2)$, where $\boldsymbol{\tau}=\boldsymbol{\tau}_1+\boldsymbol{\tau}_2$, $\boldsymbol{\tau}_1\in V_1(k, R)$, $\boldsymbol{\tau}_2\in V_2(h, R)$. Further, $\mathcal{G}(\boldsymbol{\tau})=\mathcal{G}$ if and only if $\boldsymbol{\tau}\in T_N\{G, T_G\}$. On the other hand, $\mathcal{L}^{(\alpha_1)}(\boldsymbol{\tau}_1)=\mathcal{L}^{(\alpha_1)}$ if and only if $\boldsymbol{\tau}_1\in T_N[G, T^0_{G1}]$ and $\mathcal{R}^{(\alpha_2)}(\boldsymbol{\tau}_2)=\mathcal{R}^{(\alpha_2)}$ if and only if $\boldsymbol{\tau}_2\in T_N\langle G, T^0_{G2}\rangle$. It is easy to show that the direct sum $T_N[G, T^0_{G1}]\oplus T_N\langle G, T^0_{G2}\rangle$ always contains $T_N\{G, T_G\}$. Let $\boldsymbol{\mu}_i$ be the representatives in corresponding coset resolution. Then the groups $\mathcal{G}^{(\alpha)}(\boldsymbol{\mu}_i)$ are distinct space groups while $\mathcal{L}^{(\alpha_1)}(\boldsymbol{\mu}_i)=\mathcal{L}^{(\alpha_1)}$, $\mathcal{R}^{(\alpha_2)}(\boldsymbol{\mu}_i)=\mathcal{R}^{(\alpha_2)}$.

Discussion

Factorization of reducible space groups by their partial normal translation subgroups and the inverse construction of reducible space groups as extensions of these partial translation subgroups by corresponding subperiodic groups appear to be very important and useful procedures. If we may permit ourselves to put the cart before the horse for a while, then we can suggest the following ramifications of the theory:

1. We have a new tool for construction of higher-dimensional space groups from lower-dimensional ones. As we have already said in the first part of the paper, reducible space groups can be expressed as subdirect or multiple subdirect products of lower-dimensional space groups (Kopský, 1988*a*). Another way, connected with this, is to construct higher-dimensional space groups *via* subperiodic ones. The latter can be constructed from lower-dimensional space groups and can then be used themselves for construction of higher-dimensional ones.

2. Reducible space groups are useful in the practical solution of a problem for which we suggest the name '*scanning*' of subperiodic symmetries. This can be formulated as follows: Given a space group $\mathcal{G}$ and an orientation $V_1(k, R)$ of a set of hyperplanes $(P+\boldsymbol{\tau}_2;\ V_1(k, R))$, find the subperiodic groups containing those elements of $\mathcal{G}$ which leave the hyperplanes invariant. The practically important case is the scanning of layer and rod groups. Layer symmetries in crystals, associated with certain directions of planes, are of use in the theory of domain walls and twin boundaries or even of plane defects; *i.e.* generally in problems of bicrystallography. Analogously, rod groups are useful in consideration of linear defects. Classification of layer and rod symmetries at certain locations of planes and lines can be performed in a way analogous to the classification of Wyckoff positions for site-point symmetries (Janovec, Kopský & Litvin, 1988). Reducible space groups play an intermediate role in such a determination as the so-called '*scanning groups*'.

3. The fact that subperiodic groups are factor groups of space groups can be used in representation theory. For example, the ordinary three-dimensional space groups, with the exception of cubic ones, have layer and rod groups as factor groups. In accordance

with this, each representation of a rod and/or of a layer group engenders a certain representation of all those space groups which belong to corresponding layer and rod classes. This is a suitable regularity for systemization of representations (Kopský, 1988*b*). Accordingly, there also exists isomorphism of lattices of subgroups of subperiodic groups and of sublattices of 'partially equitranslational' subgroups in the lattices of subgroups of corresponding space groups (Kopský, 1987). This relationship is quite analogous to that between the lattices of subgroups of point groups and lattices of equitranslational subgroups of space groups as given by Ascher (1968).

Reducibility can also be introduced for the subperiodic groups themselves; this can be done for ordinary as well as for contracted subperiodic groups (Litvin & Kopský, 1987). As we can see, there are many viewpoints which have to be considered in connection with the extension of the reducibility concept to the Euclidean motion groups. Points 2 and 3 show the usefulness of the concept of reducibility and of the classification of space groups into subperiodic classes even on the level of groups up to three dimensions. Such a classification has been performed and will soon be published.

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Theoretical Considerations on Two-Beam and Multi-Beam Grazing-Incidence X-ray Diffraction: Nonabsorbing Cases

BY HSUEH-HSING HUNG AND SHIH-LIN CHANG

Department of Physics, National Tsing-Hua University, Hsin-chu, Taiwan 30043

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Abstract

Two-beam and symmetric three- and four-beam grazing-incidence X-ray diffraction (GIXD) by crystals without absorption are studied based on the dynamical theory of X-ray diffraction. For two-beam cases, a new geometrical scheme is given to reveal graphically the excitation of the dispersion surface. For symmetric three- and four-beam cases, the expressions for specularly reflected and forward diffracted intensities are derived analytically. Results from the numerical calculations for the diffracted intensities, the penetration depths, the coordinates of the dispersion surface and the mode excitations are also presented for two-, three- and four-beam GIXD.

1. Introduction

Grazing incidence of X-ray scattering (GIXS), suggested by Marra, Eisenberger & Cho (1979), has been used as an experimental technique for probing the structures of crystal surfaces and overlayer interfaces. Its applications have recently been reviewed in an article by Fuoss, Liang & Eisenberger (1989). Theoretically, Vineyard (1982) described GIXS with a distorted-wave approximation in the kinematical theory of X-ray diffraction. In terms of the ordinary dynamical theory of Ewald (1917) and Laue (1931), Afanas'ev & Melkonyan (1983) worked out a formulation for the dynamical diffraction of X-rays under specular reflection conditions (GIXD - grazing-incidence X-ray diffraction) and Aleksandrov, Afanas'ev & Stepanov (1984) extended this formalism to include the diffraction geometry of thin surface layers. Subsequently, the properties of wavefields constructed during specularly diffracted reflections have been discussed in more detail by Cowan (1985) and Sakata & Hashizume (1987). Meanwhile, a geometrical interpretation of GIXS based on a three-

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